Paper number 825

Source Term Flow Rate Based on Container Wall Thickness

Jeff Henrikson* and Nathan Platt

Institute for Defense Analysis, Alexandria, VA

1. SUMMARY

It is likely that all source term models overestimate saturated toxic chemical liquid source term release rates by 2 – 3 times, depending on the circumstances.

The left hand portion of Table 1 shows the experimental flow rate of a container with a tube length of 73 cm and compares that to a theoretical release with a tube length of 0 cm using the Bernoulli equation[3] (Eqn. 1), which takes gravity and pressure differences into account. The right hand portion of Table 1 shows experimentally determined flow rates based on various tube lengths. In both cases the saturated liquid flow rate is dramatically affected by the length of the tube leading from the container to the ambient atmosphere.

$$G(\frac{kg}{s\,m^2}) = C_D\sqrt{2g(P_{\tan k} - P_{amb})\rho_L} \qquad (1)$$

Equation 1 is appropriate if the liquid doesn't flash in the container or the tube, creating a choked flow condition whereupon increasing the pressure differential between the container and the ambient surroundings doesn't increase the saturated liquid flow rate. If a saturated liquid is released through a tube longer than 10 cm, it is generally understood that the fluid will partially flash and equilibrate into a stable two-phased (or fully choked) condition, resulting in a mass flow rate that can be 20 - 40% of the value given in Equation 1.

Real world containers have a wall thickness or effective tube length between 2.5 – 8 cm and don't fit neatly into the straight-edged orifice category described by the Bernoulli equation or into the long tube lengths that develop into fully developed two-phased choked flow. This paper highlights a discrepancy between real world containers and source term models, explaining the effect that a container wall thickness greater than 0 cm and less than 10 cm has on the source term flow rate of a saturated liquid, and by extension the effect it has on the chemical dispersion and human injuries.

Experimental evidence for saturated liquids released into the ambient environment suggests that the Bernoulli equation may only be applicable with a truly straight-edged orifice and that even short tubes can cause liquids to flash, creating a partially choked flow condition. The problem is that Hazard Prediction and Assessment Capability (HPAC) model developed and maintained by the United States Defense Threat Reduction Agency (DTRA) and every other source term model we encountered thus far uses the Bernoulli equation to describe saturated liquid flow and ignores the fact that real world containers have a wall thickness, which will reduce the flow rate of the fluid. Figure 1, in the associated table, gives the experimentally determined flow rates as a fraction of Bernoulli flow for various tube lengths.

Saturated chlorine is often transported by railcar, and a railcar has a 2.5 cm thick steel plate along with 10 cm of ceramic and fiberglass insulation, for a total wall thickness of 12.5 cm. Any breach in a real railcar will result in two-phased flow with a dramatically reduced mass flow rate, but current source term models assume a straight–edged container and use Equation 1 for railcar release modeling.

Taking wall thickness into account could improve the accuracy of source term models by 2 – 3 times by providing a more accurate source term flow rate. There are times when it is sufficient to bound a source term problem using the "Bernoulli equation" for liquid flow (maximum flow rate) and the "Omega method"[4] for fully developed two-phased flow (minimum flow rate). There are also times when it is important to obtain a more accurate answer to a source term problem. The arguments in favor of accounting for wall thickness in source term models are:

1. Accounting for wall thickness when modeling a saturated liquid release will give a more accurate source term release rate.

2. Monte Carlo modeling could require half the computer time if the source term flow rate were one variable rather than bounding the problem using the Bernoulli equation and the Omega method. On the other hand, even when bounding the problem is desired, an additional run with wall thickness taken

Corresponding author address: Jeff Henrikson, Institute for Defense Analysis, 4850 Mark Center Drive, Alexandria, VA 22311-1882; e-mail: jhenriks@ida.org.

into account could provide more realistic expected source term.

3. A semi-empirical equation accounting for saturated liquid release rates through a 0 – 10 cm tube already exists and has been tested against existing water, Freon-11, and Freon-12 data.

4. During an actual release, if the chemical being released was known, then using the standard wall thickness equation[5] it would be easy to calculate the thickness of the container wall in a realistic fashion and take that variable into account when modeling the source term flow rate.

2. BACKGROUND

Toxic chemical releases from industrial manufacturing facilities or transportation storage vehicles present a real danger to human health. The storage methods and their relative danger to humans are presented in Table 2.

1. Compressed gas – Low density accounts for lower mass flow rate and lower overall mass in container.

2. Liquid at ambient (sulfuric acid, nitric acid) – Mass in container is high but the flow rate is governed only by gravity. Low evaporation means a low threat to human health.

3. Subcooled saturated liquids (ammonia, chlorine) – Mass in container is high but the flow rate is governed only by gravity. Chemical flashes fairly quickly and is limited only by the heat transfer rate from the environment to the chemical.

4. Saturated liquids (ammonia, sulfur dioxide, chlorine) – Total mass is high and the flow rate is governed by gravity as well as the high pressure in the tank. The chemical flashes almost immediately into a high concentration vapor that presents a high threat to human health.

The fluid dynamic flow rate equations for compressed gases and liquids are well known. The flow rates for saturated liquids are still being discussed in the scientific community. Figure 2 is an example of a saturated water experiment presented in Sozzi[1] where a small hole was instantaneously opened near the bottom of the container. The three distinct types of mass flow rates from left to right on Figure 2 are the liquid, swell or foam, and vapor regions. The vapor region is well understood, has a low mass flow rate, and potentially doesn’t have a large impact on human casualties. The swell or foam flow rate region has a moderate mass flow rate that is not well understood, presenting a knowledge gap that should be explored. The liquid region has a high mass flow rate, presenting the most danger to humans, and so this is the area we have concentrated our efforts on.

We performed a liquid mass flow rate check on the Sozzi saturated water data presented in Figure 2 using Equation 1 and found that while the experimental flow rate out of the container was 63.5 kg/sec (140 lbs/sec), the Bernoulli equation predicted that the flow rate should have been 145 kg/sec, or 130% higher. Furthermore, the liquid flow rate data are a constant 63.5 kg/sec even though the pressure in the tank is constantly decreasing during the release. Further investigation revealed that the saturated water exited the experimental container through a venturi constricting tube that was 73 cm long. It has been fairly well established in literature that if saturated liquid is forced through a tube longer than 10 cm into the ambient atmosphere, the saturated liquid will partially flash in the tube and create a stable two-phased condition where the flow rate is choked. Choked flow means that the fluid has reached its maximum velocity in the tube and an increase in tank pressure will not affect the mass flow rate out of the tank. This choked flow revelation with the Sozzi saturated water data led us to wonder how short the tube would have to be in order to induce the beginning of a choked flow condition, which would reduce the mass flow rate by an appreciable amount.

3. LITERATURE SEARCH RESULTS

We examined 10 articles that dealt specifically with the subject of choked flow from containers using a saturated liquid compound. The literature painted a picture of uncertainty on this subject that spanned the entire spectrum, and the top results and conclusions are presented below.

3.1 Steve Hanna et al., 2010[6]

This paper suggests that the pressure difference from the container to ambient does make a difference in the mass flow rate up to a point, and once you pass that point, increasing the pressure further has no affect. Two-phased flow is established for a saturated liquid if the exit tube is greater than 10 cm in length. It is the length of the tube that determines whether the flow rate is two-phased or liquid, and not the length / diameter ratio that has been used in the past. Choked flow does not occur for a straight-edged orifice because the liquid flashes in the atmosphere after it has cleared the tank opening. The following graphs in Figure 3 were meant to demonstrate the fall off of the mass flow rate as the tube length increased. The first graph in Figure 3 on the left comes from a Fauske[7] paper published in 1985. The data for the figure was taken from a paper published by Fauske in 1965[1], which gave a more complete picture of choked flow conditions as a function of tube length.

3.2 Richardson, S.M et al., 2006[8]

This author performed straight-edged orifice experiments on natural gas and propane mixtures. The paper suggested that saturated propane didn't flash in the orifice and did not, therefore, create a choked flow condition. There is, however, limited evidence in the author's experimental data that the saturated propane did experience limited flashing. Table 3 is an excerpt from a table in the article with 38 data points. The 4 saturated propane data points highlighted had the three lowest discharge coefficient with the fourth point being the seventh lowest. The saturated propane discharge coefficients were two standard deviations below the average for all 38 data points, possibly indicating that choked flow had been initiated. The author also notes that when pure propane was mixed with 0.07 fraction of natural gas, choked flow and flashing occurred.

3.3 Yan, Y and Thorpe, RB, 1990[9]

This study examined saturated room temperature water at 20°C and 0.0234 bar that was flashed through various orifices. Choked flow occurred with all of the straight-edged orifices that were tested. The flashing pressure was actually above the vapor pressure of the water.

3.4 Fauske, HK, 1965[2]

For this study, saturated water at different temperatures was flushed through a 0.64 cm diameter straight-edged orifice with different tube lengths. The tube lengths varied from 0 – 25 cm in length. The flow rate through the tube was progressively less as the tube length increased from 0 – 5 cm, and then the flow rate was largely unaffected by an increase in tube length. The experimental results showed that saturated water flow rate is affected by a tube length as little as 0.64 – 1.9 cm.

3.5 Shahryar Khajehnajafi et al., 1994[10]

This experiment considered straight-edged orifice flow rates on saturated water and found that choked flow never occurred because the water flashed once it was through the orifice and past the ability to affect the opening. The Bernoulli equation can be used to describe any sharp-edged orifice condition. The flow rate through the orifice was reduced to 40% of the expected flow by including 4% or more steam in the flow. The study noted that two-phased flow was predominant with tube lengths greater than 12.7 cm.

3.6 Fauske, 1985[7]

Twenty years after he published his saturated water flow rate as a function of tube length, Fauske published another paper proposing an empirical equation that provided a zeroth order fit for any saturated liquid mass flow rate in the 0 – 10 cm range.

$$G\left(kg/m^2\right) \approx \frac{h_{fg}}{V_{fg}}\left(\frac{1}{NTC}\right)^{1/2} \qquad N \approx \frac{h_{fg}^2}{2\Delta P \rho_l K^2 V_{fg}^2 TC} + 10L \quad (2)$$

In Equation 2: G = mass flux, h_{fg} = heat of vaporization, V_{fg} = specific volume change, T = temperature, C = liquid heat capacity, □P = change in pressure, ρ_l = liquid density, K = discharge coefficient, and L = tube length (0 – 10 cm). Equation 2 was applied to saturated chlorine at room temperature, arriving at Figure 5. Fauske used the empirical equation he developed and compared it to the water, Freon-11, and Freon-12 data that existed at the time and found that the fit was good.

Fauske also put together a table showing the saturated fluid data that had been collected to date, and is shown here as Table 4. The orifice openings ranged from 6 mm to as much as 0.5 m.

4 REAL WORLD CONTAINTER THICKNESSES

Saturated liquid chlorine is typically transported using a standard 105J500W rail tank car. This type of railcar is regulated by government law[11] to have a shell thickness of 2.5 cm encased in 10 cm of insulation. A real world release of liquid chlorine from a railcar should not be modeled as a straight-edged release, but rather as a fully developed two-phased release.

For chlorine storage in an industrial container setting, government law[12] is again applicable. The equation to determine the wall thickness of a cylindrical pressurized container is given as Equation 3 where P = pressure, r_i = container radius, S = strength of steel, E_J = joint efficiency, and Cc is the corrosion allowance.

$$t = \frac{P\, r_i}{S\, E_J - 0.6\, P} + C_C \qquad (3)$$

Based on Equation 3, a saturated chlorine container would be 2.5 – 8 cm thick based on 1000 – 100,000 gallons chlorine. This conservative wall estimate, combined with our literature search, suggests that the Bernoulli equation may not be appropriate in some real world industrial settings.

5 CONCLUSIONS AND FUTURE WORK

The literature search that we performed on choked flow conditions for saturated liquids gave a picture that was not completely consistent. There seems to be consensus that fully developed two-phased choked flow is well established if the tube is longer than 10 cm, and that the Bernoulli equation accurately describes a straight-edged release. The modeling community has essentially ignored the region where the tube length is greater than 0 cm and less than 10 cm. Unfortunately, nearly every real world container has a wall thickness inside this region, meaning that in most cases the source term models have a potential to strongly over or under predict the mass flow rate.

The source term modeling community has focused on the two extremes where the minimum flow rate is given as fully choked and modeled with the "omega method" and the maximum flow rate is found using the Bernoulli equation. In some instances these minimum and maximum methods may be sufficient and desirable, but there are many instances where the more realistic flow rate would be desirable.

1. Accounting for wall thickness when modeling a saturated liquid release will give a more accurate source term release rate.

2. Monte Carlo modeling could require half the computer time if the source term flow rate were one variable rather than bounding the problem using the Bernoulli equation and the Omega method. On the other hand, even when bounding the problem is desired, an additional run with wall thickness taken into account could provide more realistic expected source term.

3. A semi-empirical equation accounting for saturated liquid release rates through a 0 – 10 cm tube already exists and has been proven against existing water, Freon-11, and Freon-12 data.

4. During an actual release, if the chemical being released was known, then using the standard wall thickness equation[13] it would be easy to calculate the thickness of the container wall in a realistic fashion and take that variable into account when modeling the source term flow rate.

With regards on how to proceed next, there is enough data in the literature on choked flow conditions for saturated liquids to recommend preliminary changes to HPAC and other source term models. The Simple and Detailed Industrial Facility Modules inside of HPAC already calculate a minimum wall thickness for every industrial container and the wall thickness for transportation containers is well known. The semi-empirical equation developed by Fauske could be used to estimate the mass flow rate based on a given wall thickness. Lastly, given the importance of an accurate source term, the fact that source terms for saturated liquids could be off significantly, and that saturated liquids represent the largest threat to human health, experiments could be designed using two or three compounds, orifices, and tube lengths. The results of such a study could improve the accuracy of toxic saturated liquid flow rate source terms.

ACKNOWLEDGEMENTS

This effort was supported by the Defense Threat Reduction Agency with Dr. John Hannan as the project monitor. The views expressed in this paper are solely those of the authors.

REFERENCES

1. Sozzi, G.L., "Level Swell and Void Fraction Measurements during Vessel Blowdown Experiments, Data Set No. 21," Multiphase Science and Technology. Vol. 6, p. 167 – 211, 1992.

2. Fauske, H.K., "The Discharge of Saturated Water Through Tubes," Chem. Eng. Prog. Symp. Series, Vol. 61, No. 59 (1965).

3. Felder, R.M and Rousseau, R.W. Elementary Principles of Chemical Processes, 2nd Edition. John Wiley & Sons, New York. 1986.

4. Leung, J.C. "A generalized correlation for one-component homogeneous equilibrium flashing choked flow." AIChE Journal, 32, 1743-1746. 1986.

5. Peters and Timmerhaus. Plant Design and Economics for Chemical Engineers, 4th edition. McGraw Hill, pp. 536, 1991.

6. Hanna, S. et al. "Toxic Industrial Chemical (TIC) source emissions model improvements for pressurized liquefied gases", 2010, (in press).

7. Fauske, H.K.. "Flashing flows or: some practical guidelines for emergency releases." Plant/Operations Progress, vol. 4, pp. 132-134, 1985.

8. Richardson, S.M. et al. "Experimental determination of two-phase flow rates of hydrocarbons through restrictions." Process Safety and Environmental Protection. Trans I Chem E Part B. 84(B1), 40-53, 2006.

9. Yan, Y and Thorpe, RB. "Flow Regime Transitions Due to Cavitation in the Flow Through an Orifice." Int. J. Multiphase Flow Vol. 16, No. 6, pp. 1023 – 1045, 1990.

10. Khajehnajafi, S and Shinde, A. "Prediction of discharge rate from pressurized vessel blowdown through sheared pipe." Process Safety Progress. Vol. 13, Issue 2 , pp. 75 - 82, 1994.

11. "Predicted Damage to a Chlorine Rail Tank Car from Selected Threat Weapons," 2008.

12. The ASME Boiler and Pressure Vessel Code, American Society of Mechanical Engineers, New York City, Section VIII.

13. Peters and Timmerhaus. Plant Design and Economics for Chemical Engineers, 4th edition. McGraw Hill, pp. 536, 1991.

Sozzi Exp Data		
Length of Tube (cm)	0	73
Liquid Flow Rate (kg/s)	358	161
Time of Liquid Release (hrs)	1.4	2.9
AEGL Area 1 (Death)	7.2	6.9
2 (Injury)	172	89
3 (Symptoms)	2257	714

Fauske Exp Data				
Length of Tube (cm)	0	0.64	2.54	25.4
Liquid Flow Rate (kg/s)	358	304	226	104
Total Dispersion Time (hrs)	1.0	1.0	1.0	1.0
AEGL Area 1 (Death)	8.6	5.9	4.7	2.4
2 (Injury)	80	75	68	35
3 (Symptoms)	110	105	99	87

Table 1: Sozzi[1] and Fauske[2] experimental saturated water flow rate data compared against various tube lengths

Threat Comparison of Toxic Chemical Storage Methods				
	Mass in Container	Mass Flow Rate	Airborne Threat	Use in Industry
Compressed Gas	Low	Low	High	Low
Ambient Liquid	High	Medium	Low	High
Subcooled Liquid	High	Medium	Medium	Medium
Saturated Liquid	High	High	High	High

Table 2: The human risk associated with each chemical storage method

Diameter (mm)	Pressure (bara)	Temperature (C)	Propane mass frn	Total flow rate (kg s^{-1})	Liquid mass fraction		Discharge coefficient
					Post-equilibn	In throat	
7	6.3	9.1	1.000	0.505	1.000	1.000	0.567
7	8.7	9.7	1.000	0.632	1.000	1.000	0.585
7	11.7	9.9	1.000	0.744	1.000	1.000	0.586
7	14.5	10.3	1.000	0.840	1.000	1.000	0.588
7	19.9	10.7	1.000	0.996	1.000	1.000	0.589
10	6.5	10.3	1.000	1.041	1.000	1.000	0.579
10	6.4	9.7	1.000	1.009	1.000	1.000	0.566
10	6.6	10.5	1.000	1.069	1.000	1.000	0.586

Table 3: Discharge coefficients of liquid propane as it passes through a straight-edged orifice[8]

Table 1. Minimum pressure at choked and super cavitation

d (cm)	P_2(bar)
1.52	0.0281 ± 0.0000
1.72	0.0300 ± 0.0008
2.02	0.0290 ± 0.0011
2.32	0.0292 ± 0.0004
2.50	0.0298 ± 9.0014
2.72	0.0289 ± 0.0007

Table 4: Pressure at which room temperature water reached fully developed two-phased choked flow with various straight-edged orifices[7]

Critical Flow Experiments with Flashing Liquids					
Source	Material	D (mm)	L/D	L (mm)	Pressure (bar)
Fauske	Water	6.35	~16	~100	34, 102
Ogasawara	Water	10.9, 32.9, 50.5			9, 60, 67
Sozzi and Sutherland	Water	12.7	~10	~127	65.6
Kevorkov et al.	Water	14, 25, 37.8			3, 10, 40, 90
Marviken	Water	500	> 0.33	> 166	50
Flinta	Water	35	~3	~100	
Uchida and Nariai	Water	4	~25	~100	
Fletcher	Freon-11	3.2	~33	~105	
Van Den Akker	Freon-12	4	~22	90	

Table 5: Flow rate experiments with flashing liquids and varying tube lengths

Tube Length (cm)	% of Bernoulli Flow	Length / Diameter
0	100	0
0.6	85	1
1.3	78	2
1.9	73	3
2.54	63	4
25	29	40

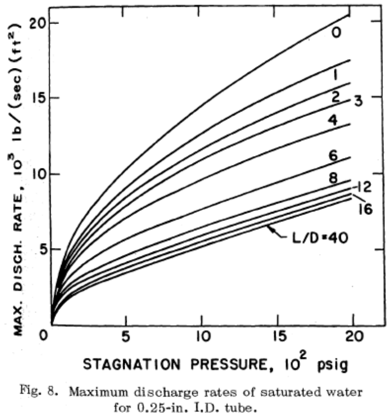

Figure 1: Mass flow rate results for saturated water using various tube lengths[2]

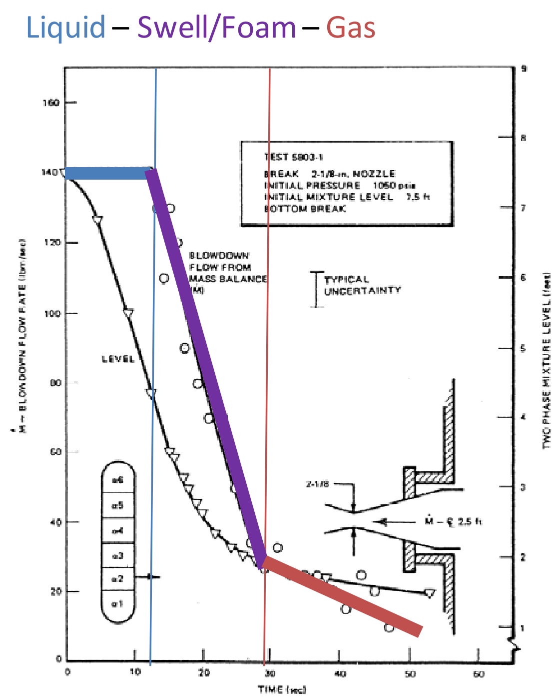

Figure B-11: Blowdown response for large blowdown vessel test 5803-1

Figure 2: Saturated water container release data from Sozzi[1] paper

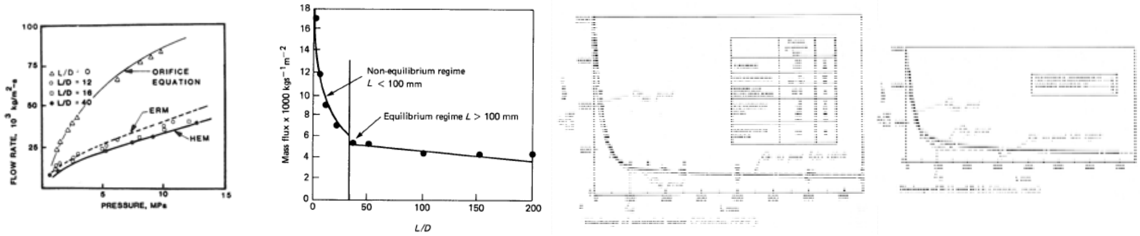

Figure 3: Transition from straight-edged Bernoulli mass flow rate to fully developed two-phased choked mass flow rate

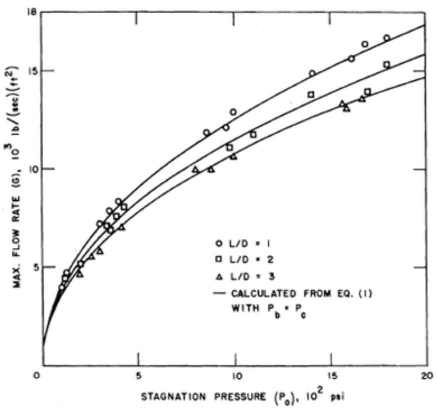

Fig. 4. Maximum discharge rates of saturated water for 0.25-in. I.D. tube.

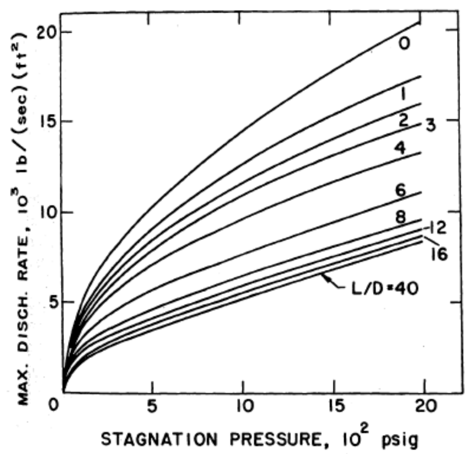

Figure 4: Graphs from the article showing that small tube lengths impact mass flow rate

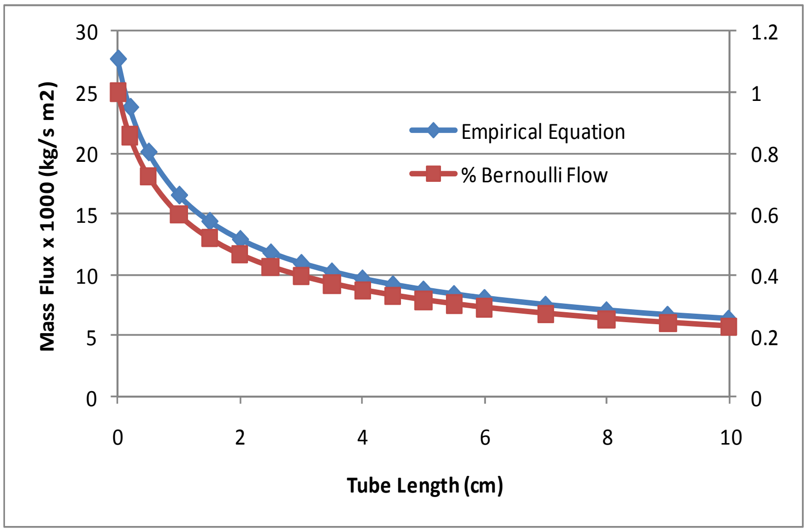

Figure 5: Theoretical saturated chlorine flow rate when the tube length is between 0 – 10 cm

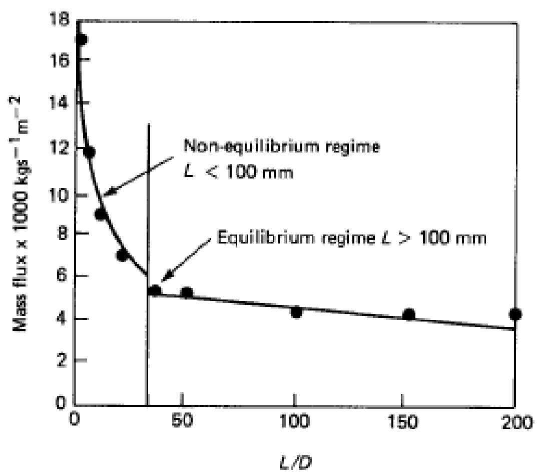

Figure 6: Empirical equation fit with experimental Freon-11 data